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EINLADUNG zum IFP-SEMINAR

Approach to large cluster problems: Cellular dynamical mean field theory combined with real-space renormalization

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Host:	Karsten Held
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Strong correlation effects generate various phenomena, such as the Mott metal-insulator transition and high-temperature superconductivity. One of the useful methods widely explored in correlated models to study these phenomena is cellular dynamical mean field theory (CDMFT) [1], which solves a lattice model by mapping it onto a cluster impurity model coupled to a fermionic bath. However, the CDMFT simulations with a large cluster have been a numerical challenge since the computational cost rapidly increases with the cluster size.

We propose a real-space renormalized DMFT (rr-DMFT) [2] as an approach to solve large cluster problems efficiently. The rr-DMFT solves a large cluster model by decomposing and mapping it onto multiple small cluster problems where we trace out sites with a real-space renormalization. The computational cost is considerably reduced by this procedure in comparison with the CDMFT. We benchmark the rr-DMFT in the two-dimensional Hubbard model on a square lattice through calculating the self-energy, spin structure factor, density of states and the Mott metal-insulator transition and show its improved efficiency and accuracy.

[1] G. Kotliar, S. Y. Savrasov, G. Pálsson, and G. Biroli, Phys. Rev. Lett. 87, 186401 (2001).
[2] D. Kubota, S. Sakai, and M. Imada, Phys. Rev. B 93, 205119 (2016).